

Topic Paper #6

Low Temperature Combustion

On August 1, 2012, The National Petroleum Council (NPC) in approving its report, *Advancing Technology for America's Transportation Future*, also approved the making available of certain materials used in the study process, including detailed, specific subject matter papers prepared or used by the study's Task Groups and/or Subgroups. These Topic Papers were working documents that were part of the analyses that led to development of the summary results presented in the report's Executive Summary and Chapters.

These Topic Papers represent the views and conclusions of the authors. The National Petroleum Council has not endorsed or approved the statements and conclusions contained in these documents, but approved the publication of these materials as part of the study process.

The NPC believes that these papers will be of interest to the readers of the report and will help them better understand the results. These materials are being made available in the interest of transparency.

Low Temperature Combustion – A Thermodynamic Pathway to High Efficiency Engines

David E. Foster
Phil and Jean Myers Professor
Engine Research Center
University of Wisconsin – Madison

Prepared for the National Petroleum Council Fuels Study

March 2012

Abstract

This article makes the argument that compression ignition combustion processes that are “flameless” with volumetric energy release, described as Low Temperature Combustion (LTC), are a thermodynamic pathway to maximizing the efficiency of reciprocating piston, internal combustion engines. The argument is built from the foundation of determining the maximum theoretical efficiency for an IC Engine and then identifying the irreversibilities associated with the various in-cylinder processes. Low Temperature Combustion minimizes the sum of the irreversibilities for work generation from in-cylinder processes. The underlying objective of Low Temperature Combustion is to keep in-cylinder temperatures low through volumetric energy release via auto-ignition of dilute air fuel mixtures, as opposed to flame propagation. Because LTC depends on auto-ignition, the methods used to achieve it are dependent on the auto-ignition characteristics of the fuel being used. Differences in physical and auto-ignition characteristics of fuels mandate different approaches for establishing and controlling LTC. It has become common to label the different approaches with a descriptive acronym, leading to a proliferation of terms such as HCCI, PCCI, CAI, etc. Because the energy release is volumetric it is a challenge to operate at low loads with good combustion stability, and at high loads without excessive rates of pressure rise. Good progress is being made addressing these challenges but doing so will put added burden on the gas exchange and control systems of the engine.

Introduction

Internal combustion engines using liquid hydrocarbon fuels are an extremely effective combination of energy converter and energy carrier for mobility applications. The high energy density and specific energy of liquid hydrocarbons are well matched for applications in which the fuel must be carried onboard the vehicle; and the engine is a convenient and effective device for converting the stored energy in the fuel into mobile power. Together the IC Engine and HC fuel are a robust and economically viable power propulsion system and will remain so for decades to come [1]

However, the principle source of fuel – petroleum, is a limited resource which is in high demand and with the global development currently underway the demand is likely to

increase. Furthermore the impact of carbon emissions from our mobility systems is a concern relative to its impact on the global climate. Consequently, it is important that our mobility systems achieve the maximum possible efficiency with minimal environmental impact, while still preserving utility to the user. And, this must be done as the diversity of the feedstock of our fuel supply increases. In the author's opinion this is one of the grand challenges facing the propulsion technical community today.

Two reasonable questions arise when considering the powertrains of our propulsion systems. What is the maximum efficiency that is theoretically possible and how does the efficiency of our current powertrains compare to this maximum? And secondly, what are practical limits to the efficiency when realistic engineering constraints are imposed on the system? This latter question is very important in that it yields realistic stretch targets to which we direct our development efforts, and it allows us to identify the important phenomena that should be addressed to make our mobility systems consume less fuel, emit little to no emissions, and still provide the desired utility.

Of IC Engines in use today the diesel, or compression ignition engine, is the most efficient at converting fuel energy to shaft work. This article will describe a combustion process, that builds on the inherent advantages of diesel combustion, which the author believes offers a pathway to achieving maximum practical efficiency from a reciprocating piston IC Engine – Low Temperature Combustion (LTC). To do this I will first review the maximum theoretical efficiency for an internal combustion engine and then identify the losses which occur in a typical engine. From this perspective I will offer discussion as to which losses are unavoidable and comment on how LTC results in the minimum sum of losses for in-cylinder processes during conversion of fuel energy to work. This will be followed by a general overview of the different ways in which LTC can be achieved, which is strongly dependent on the ignition characteristics of the fuel, or fuels, being used. The challenges of operating LTC over the entire load range of the engine and engine system issues will also be briefly discussed.

Maximum Possible Work

One of the most important concepts to realize when asking what is the maximum possible work that can be obtained from an internal combustion engine is that the engine we use in our propulsion systems does not undergo a thermodynamic cycle. It is a chemical process. In a thermodynamic cycle the working fluid undergoes a cycle. This does not happen in an internal combustion engine. The air fuel mixture is brought into the engine, prompted to react to products, expanded, and then exhausted. The next engine cycle uses a different air fuel mixture; the working fluid is thrown away and not brought back to its initial state. Consequently, using classic thermodynamic heat-engine cycle analysis is not appropriate to answer the questions being addressed.

A thermodynamic analysis describing the maximum useful work that can be obtained from a chemical process, such as the combustion process in an internal combustion engine, shows that the maximum useful work obtainable is the negative of the change in Gibbs Free Energy of the chemical reaction, (equation 1) [2]:

$$W_{\max, \text{useful}} = -(\Delta G)_{T_0, P_0} \text{ Eq. 1}^{12}$$

It is instructive to conceptualize what an internal combustion engine would look like if it could be made to achieve this ideal result. Figure 1 is such a conceptualization. The embodiment of the ideal engine shown in Figure 1 appears to be similar to what is actually in development today. However, there are distinct pedagogical differences. In the conceptualization shown in Figure 1, it is assumed that everything is reversible in the engine. Namely the air and fuel enter the engine at atmospheric temperature and pressure, undergo reversible processes throughout the engine, including the chemical reaction, and then leave the engine as equilibrium products at atmospheric conditions. Mandating reversible processes will dictate specific state histories so it may be necessary to invoke heat transfer to get the products to atmospheric temperature. As depicted in the figure, any such heat transfer would be done through a reversible heat-engine which has its heat rejection at atmospheric temperature. The work obtained from this reversible heat-engine is then added to the work output of the engine shaft to give the maximum possible work.

Shown on the bottom of Figure 1 is the energy balance for determining the work from this reversible engine. Note that the maximum work theoretically obtainable is equal to the heating value of the fuel, Q_{HV} , adjusted by the unusable heat which is rejected at atmospheric temperature, $T_0 * (S_{prod} - S_{react})$. The combination of these two terms is equal to the negative of the change in the Gibbs free energy of the chemical reaction, equation 1.

¹ In this presentation I am being imprecise in the way I am reporting the change in Gibbs free energy. I do not include work that could have been obtained by allowing the individual components of the combustion product mixture to equilibrate to the partial pressures at which they exist in the ambient. Including this work would result in an increase in the maximum theoretical work reported here. This increment is a relative small number and not including it keeps the discussion more concise and does not change the thrust of the assessment presented.

² As an aside, it is worth noting that this is also the equation for the maximum theoretical useful work that can be obtained from a fuel cell. When describing a fuel cell it is usual to write:

$$(\Delta G)_{\text{rxn}} = -nFE$$

where:

n = number of moles of electrons transferred
 F = Faraday's constant
 E = Electrical potential difference

When expressing the Gibbs free energy in above equation in terms of electrochemical potentials it is called the Nernst Equation [3]. The maximum theoretical work from an internal combustion engine and from a fuel cell is given by the same equation.

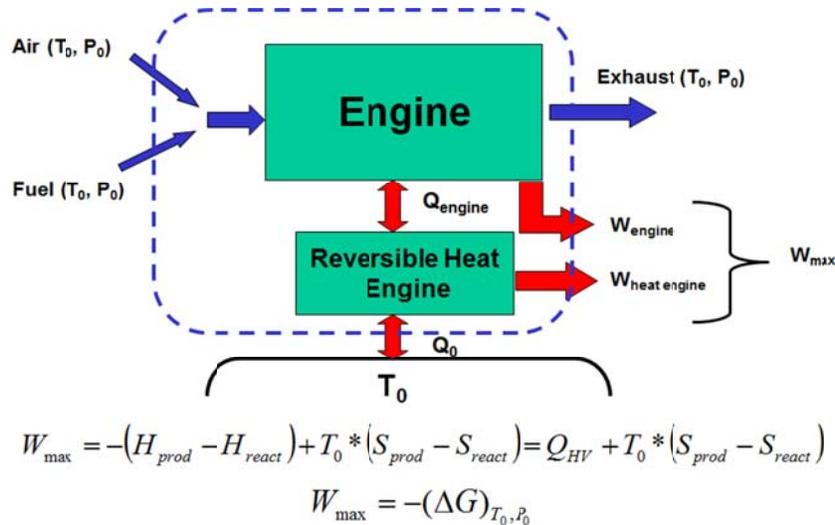


Figure 1, Conceptualization of an Engine to Achieve the Maximum Possible Work from a Charge of Air and Fuel Reacting to Products

The Relationship between the Fuels Heating Value and Gibbs Free Energy

One interesting subtlety of this result is the realization that the maximum theoretical work obtainable from an internal combustion engine, or fuel cell, is given by the change in Gibbs free energy as opposed to the fuel's Heating Value. A table comparing the Heating Value and the negative of the Gibbs free energy for several fuels when oxidized with air at atmospheric conditions is shown below.

Table 1 Enthalpies and Gibbs free energy changes of several fuels when reacted with air at atmospheric conditions (adapted from Heywood [2])

Fuel	Heating Value (MJ/kmol)	- Gibbs Free Energy (MJ/kmol)
Methane	802.3	800.6
Methanol	638.59	685.35
Propane	2044.0	2074.1
Octane	5074.6	5219.9

Two observations are apparent in examining the values given in Table 1. First the Heating Values and changes in Gibbs free energy of reactions for typical hydrocarbon fuels are very close to the same value. That is the maximum theoretical efficiency of an internal combustion engine is effectively one hundred percent. The second observation is that some of the changes in Gibbs free energy have a larger magnitude than the Heating Value. This indicates that theoretically it is possible to extract more work from the engine than the heating value of the fuel, which is typically referred to as the energy input. This circumstance is a result of isentropic expansion of the products of combustion all the way to atmospheric pressure as part of maximizing the work output. In some cases, following the isentrope to atmospheric pressure would result in a temperature below atmospheric, which means that the heat transfer between the engine and the environment

is from the environment to the engine. Thus work would be obtained from the auxiliary reversible heat-engine through a heat transfer from the environment into the engine to bring the engine back up to the atmospheric temperature.

For the purpose of the discussion which follows I will take the maximum theoretical efficiency of an IC engine to be 100 percent, and not dwell on the subtlety of the differences between the Gibbs free energy and the Heating Value of typical hydrocarbon fuels.

Identifying Irreversibilities within the Engine

There are two underlying precepts in understanding the maximum theoretical work that could be obtained from an internal combustion engine. The first is that all processes are conceptualized to be reversible. That is, all of the energy within the fuel that could have been converted into useful work actually is converted into useful work. This recognizes the second precept underlying the development, namely that energy has quality, called exergy or availability, and that irreversible processes degrade useable energy into unusable energy; namely exergy or availability destruction. Evaluating the availability destruction that occurs in the processes of a real engine is an instructive exercise for quantifying losses relative to the ideal engine described above. Furthermore it is possible to assess whether technological development can make inroads into reducing those losses and thus improving the efficiency of the engine. An analysis of the losses is brought about by performing an availability, or exergy, balance. Such a balance is shown in Figure 2.

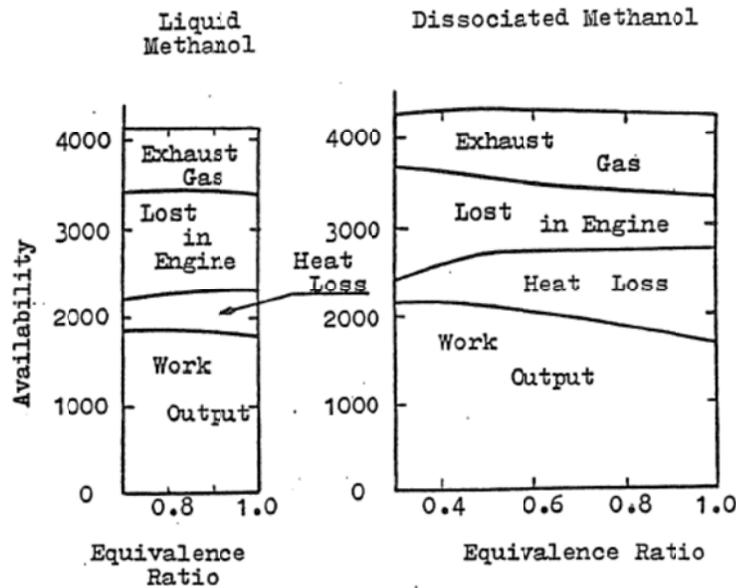


Figure 2, Availability Accounting per Unit of Fuel for Engine Operation at Different Equivalence Ratios for Methanol and Dissociated Methanol [4]. (Units on the ordinate are kcal per liter of methanol)

The graphs given in Figure 2 are displayed in terms of availability, expressed as kcal/liter of CH₃OH. The plots are really stack charts showing the partitioning of the available energy of the fuel among the different energy flows associated with the engine at each equivalence ratio. The area under the bottom line on each graph is the work output of the engine. This is the portion of the available energy that was converted to work and when expressed as a ratio with the heating value of the fuel gives the efficiency of the engine at that operating point. The other regions on the graphs show the available energy of the fuel that did not leave the engine as work, and as such represent a loss. The plots show that a significant fraction of the fuel energy that could have theoretically been converted to work is degraded into non useable forms, i.e. an availability destruction or “loss”. The energy is conserved but its usability has been degraded.

Figure 2 shows what happens to the useable energy for each operating condition. The work output represents energy leaving the engine as shaft work, the desired outcome for the engine. The heat loss represents useable energy that left the engine as a heat transfer as opposed to shaft work. The term “lost in engine” is a measure of the irreversibilities of the combustion process itself. It is not an inefficiency of combustion. It is a degradation of useable energy because of the unconstrained chemical reactions taking place within the combustion chamber, even though the combustion has gone to completion. Finally, the exhaust gas availability is the useable energy leaving the engine in the exhaust. The available energy contained within the heat transfer and exhaust gases leaving the engine represent that portion of the energy in the heat transfer and exhaust flow that is useable, as opposed to the amount of energy within those respective flows.

Several observations can be made from Figure 2. First, there is a significant irreversibility associated with the combustion process and this loss gets bigger when the engine is operated under lean conditions. This loss represents approximately 20 percent of the fuel’s useable energy. Second, there are significant available energy flows leaving the engine in the form of heat transfer and exhaust flow. And finally, the work out of the engine per unit of fuel increases for lean mixtures, even though the irreversibilities of combustion increases. This is so because the available energy thrown away in the exhaust and with the heat transfer decreases as the engine is operated with progressively leaner air-fuel ratios. These decreases more than compensate for the increased losses that occur within the lean combustion. This trade-off is an important component of maximizing engine efficiency and achieving it has close ties with the characteristics of the fuel.

Detailed Analysis of the Individual Losses

A more detailed assessment of the individual losses is insightful as to where potential for improving the efficiency of real engines lie. As a prelude to this discussion I point out that the analysis of the losses presented in Figure 2 did not include engine friction, or pumping work. Indeed, reduction in engine friction and pumping work is an important component of improving efficiency. Friction represents work that was leaving the engine as shaft work but got diverted. Pumping work is work leaving the engine as shaft work that must be returned to exchange the gases in the cylinder. Any reduction in these two

work quantities manifests itself immediately as a one-to-one increase in shaft work. For engine system efficiency, any changes made in-cylinder to increase the engine efficiency must be weighed against the impacts such changes have on the required pumping work and the resulting friction.

Availability Destruction from Combustion

A loss of approximately 20 percent of the fuel's useable energy in combustion is discouraging and would seem to represent an opportunity for improvement. This has been the subject of much discussion and analysis [5, 6, 7, and 8]. However, the combustion irreversibility is a result of allowing the gradient between chemical potentials of the reactants and products, the affinity, to relax unconstrained. Thermodynamics teaches us that when any large gradient is allowed to relax unconstrained there will be large losses, viz. heat transfer across a large temperature gradient, or the irreversibilities associated with fluid flow driven by a large pressure gradient. Even if it were possible to extract work from the cylinder at the same rate at which the chemical reaction were occurring – constant temperature combustion, the irreversibilities of combustion would not be reduced [9]. The only way to reduce the irreversibilities of combustion is to raise the temperature at which the chemical reactions occur. This is why the losses of combustion increase with lean operation, the combustion temperatures are lower. Within the practical combustion temperatures for internal combustion engines the irreversibilities of combustion will range from 20 to 25 percent [9].

Consequently, using combustion - unconstrained chemical reactions, as part of the process of converting the chemical energy of the fuel into work, results in a loss of approximately 20 to 25 percent of the work potential of the fuel. We will not be able to engineer our way around this³.

The paradox of increased combustion irreversibilities and increased work output per unit mass of fuel with lean combustion is resolved through a more detailed assessment of the availability transfers occurring during the expansion process, which impacts the availability leaving the engine in the exhaust gas and as heat transfer.

Work Extraction via Cylinder Gas Expansion and Useable Exhaust Energy

It is common practice to plot the pressure and volume history during compression and expansion on logarithmic coordinates. When this is done we find that the slope of the log P, log V plot is very closely equal to the ratio of specific heats of the gases in the cylinder, γ . This means that for the gases in the cylinder the compression and expansion process are very nearly reversible. Compression and expansion within the engine are very efficient. The work obtained from the gases being expanded within the cylinder is given by the expression:

$$w = \int Pdv$$

³ It is worth noting that this same analysis is also true for fuel cells.

The pressure and the volume are related via the expression:

$$Pv^\gamma = \text{constant}$$

where:

w = work per unit mass

P = cylinder pressure

v = specific volume of the gases in the cylinder

γ = ratio of specific heats

The ratio of specific heats, which is a function of gas composition and temperature, plays an important role in determining the work output from the engine.

Figure 3 is a simple plot showing the effect of composition and temperature on the ratio of specific heats, γ , and the impact of the value of γ on the engine efficiency. In the Figure one can see that as the temperature increases, γ decreases. It is also apparent that at a given temperature γ is lower for a mixture of combustion products than it is for air. This will also be true for combustion products relative to the air fuel mixture of the reactants before combustion. The right hand plot shows the efficiency of an engine at different compression ratios for different values of γ^4 . From the two graphs in Figure 3 it is evident that if γ is larger there is more work extraction per unit of volume expansion in the engine. Furthermore it is apparent that small changes in γ can have measurable impact on the efficiency.

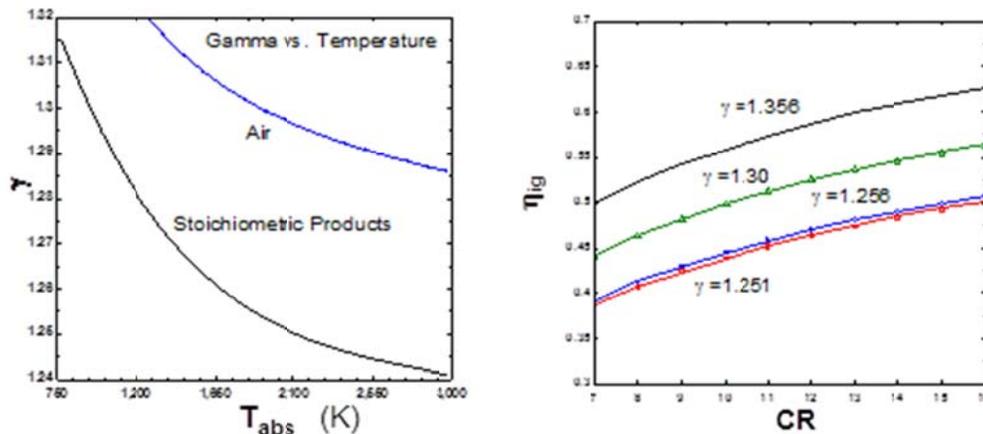


Figure 3, The Effect of Mixture Composition and Temperature on γ , and the Effect of γ on the Efficiency of an Internal Combustion Engine – Plotted vs. Compression Ratio (CR)

Herein lays one of the reasons for the higher efficiency of lean burn engines. Lean burn engines have lower combustion temperatures than stoichiometric engines. Even though

⁴ For ease of presentation the calculation of the efficiency shown here was done using a simplified ideal gas analysis.

there is a decrease in γ because of the composition change and the increase in temperature from combustion, the lower temperature of the lean combustion results in a γ that is larger compared to that for the stoichiometric combustion products. The larger relative γ of lean combustion results in a larger work extraction per increment of volume expansion than occurs with stoichiometric combustion. Because of this there is less useable energy thrown away in the exhaust with lean combustion. This is what was shown in Figure 2. The same effect is also seen with dilute combustion.

An important avenue for increased work output per unit of volume expansion is to keep temperatures in the combustion chamber low. However, as a combustible mixture is made lean or dilute the rate at which a flame propagates slows. In practical applications lean, or dilute, combustion via flame propagation will have extended combustion duration which works against efficiency. To reap the benefit of lean combustion one must also maintain short combustion durations. The fuel plays an important role in achieving this goal.

Useable Energy in the Heat Transfer

The available energy in heat transfer depends on the quantity of heat transfer and the temperature at which the heat transfer takes place. Heat transfer occurring at higher temperatures has the ability to do more useful work than lower temperature heat transfer.

Figure 4 shows the heat transfer availability, the portion of the heat transfer that could theoretically be converted to work, as a function of the temperature at which the heat transfer takes place. The range of temperatures shown in the Figure was chosen to represent temperatures that might typically be experienced during combustion.

As the temperature at which the heat transfer takes place increases a larger portion of the heat transfer energy has the capacity to be converted into work. The two illustration lines on the Figure show the portion of the heat transfer energy that could be converted into useful work for heat transfer occurring at temperatures of 2600 K and 1900 K respectively. These temperatures could be considered representative of those occurring during stoichiometric and dilute combustion. Each unit of heat transfer at 2600 K has approximately 3 percent higher availability than a similar unit of heat transfer at 1900 K. That is each unit of energy lost to heat transfer at 2600 K represents a 3 percent greater loss of work potential than the same quantity of heat transfer lost at 1900 K.

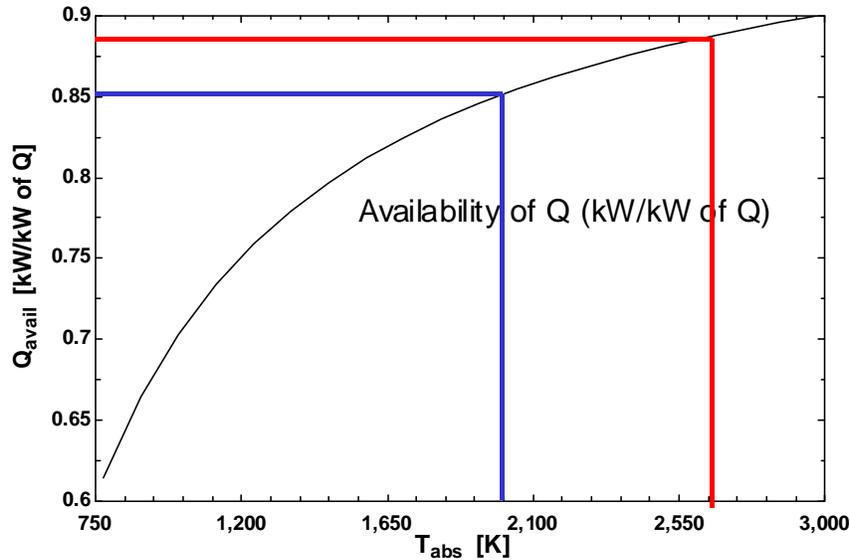


Figure 4, Proportion of the Heat Transfer that Could be Converted into Useful Work vs. Temperature at which the Heat Transfer Takes Place.

There is an added subtlety. The rate of heat transfer is proportional to the temperature difference driving it. The lower in-cylinder temperatures associated with low temperature combustion results in a lower driving potential for heat transfer. Lower in-cylinder temperatures reduce both the quantity of heat transfer and the work potential of each unit of that heat transfer.

Overview of the Fundamentals of IC Engine Efficiency and Losses

Through the discussion presented above it has been shown that for purposes of assessing the maximum theoretical efficiency of an internal combustion engine running on hydrocarbon fuels, one can essentially consider all of the energy in the fuel to be available to do work. The maximum theoretical efficiency of an internal combustion engine is 100 percent.

However, because we use an unconstrained chemical reaction as part of the energy conversion process approximately 20 to 25 percent of the fuel's available energy is destroyed. As long as unrestrained chemical reaction is used in our propulsion systems within current combustion temperature ranges, this loss is unavoidable.

Reducing the loss of work potential associated with heat transfer and exhaust gas leaving the engines is doable. To this end, efforts which minimize the reduction in γ from combustion help to maximize the work extraction per unit of volume expansion, which increases efficiency and results in less usable energy being thrown away in the exhaust. Minimizing the reduction in γ can be achieved by keeping in-cylinder combustion temperatures as low as possible, even though this results in slightly larger combustion irreversibilities.

In addition lower in-cylinder temperatures also have a beneficial effect on heat transfer losses. Not only does the magnitude of heat loss decrease with lower in-cylinder temperatures, but the proportion of that energy that has the capacity to be converted into work is also reduced.

Low Temperature Combustion

Originally, the interest in low temperature combustion (LTC) was motivated by the desire to reduce emissions, mainly NO_x and particulate matter (PM). However, we now understand that there is an additional motivation to pursue low temperature combustion that is at least of equal value to reducing emission, reducing fuel consumption.

As one attempts to continually reduce the combustion temperature flame propagation becomes a problem and ultimately limits engine operation. However, if combustion is achieved via auto-ignition of a dilute mixture the energy release becomes volumetric and can be achieved in an acceptable crank-angle interval, even for mixtures which would not support flame propagation. One can think of this as moderated knock. Rather than a flame propagating through the mixture, the entire mixture auto-ignites. The energy release is distributed throughout the volume of the combustion chamber as opposed to being localized within a flame. Locally the chemical reaction is slow, because the temperatures are low, but because the energy release is distributed throughout the combustion chamber volume the integrated heat release rate can be made to match or surpass that obtained from flame induced energy release. For conciseness one can say the combustion is “flameless”, or the energy release is volumetric. To achieve this requires very different control of in-cylinder conditions relative to typical flame driven energy release. This is what I refer to generically as low temperature combustion, LTC.

LTC is in essence controlled knock, and relies on the auto-ignition chemistry of the fuel. Regardless of the fuel, the underlying approach to achieving acceptable LTC is the same. One wants to get the fuel vaporized and partially mixed with the cylinder gases such that when the auto-ignition chemistry reaches the point of ignition the energy release is volumetric. Furthermore there needs to be sufficient inhomogeneity of the mixture within the combustion chamber that the entire mixture does not auto-ignite all at once, which leads to excessive rates of pressure rise. This inhomogeneity can be in temperature, air fuel ratio, or degree to which the local mixtures have kinetically traversed their auto-ignition pathway. There needs to be a propagation of ignition through the mixture, where a few locations auto-ignite first which then induce other regions to auto-ignite which in turn induce others. It is an ignition propagation process and not a flame propagation process. Depending on the volatility and ignition characteristics of the fuel, the pathway to achieving this can be very different.

For example, gasoline-like fuels vaporize easily and have long ignition delay times, so getting the mixture to auto-ignite at the desired time is more of a challenge than getting the fuel to vaporize and mix with the cylinder gases. Typically cylinder temperatures at IVC to achieve LTC with gasoline like fuels will be higher than those required for LTC with diesel like fuels. A diesel like fuel with lower volatility and short auto-ignition

times mandates an operational strategy to achieve LTC which is vastly different than for gasoline like fuels; typically a very early injection is required to allow time for vaporization and mixing, and because of the rapid auto-ignition rates a low temperature and low oxygen concentration – high EGR which is aggressively cooled, are necessary to stretch out the ignition delay as much as possible.

Depending on the details of the fuel structure, the auto-ignition chemistry will have different levels of sensitivity to in-cylinder pressure and temperature histories. For example the LTC operating regimes for iso-octane and ethanol will be different and have different responses to changes in an engine’s operating condition even though the two fuels have high octane numbers.

The alphabet soup of acronyms that has arisen, HCCI, PCI, PPCI, CAI, RCCI, etc. to describe the different approaches for achieving low temperature combustion signify the different ways researchers are choosing to establish and control the basic requirements for this “flameless” combustion.

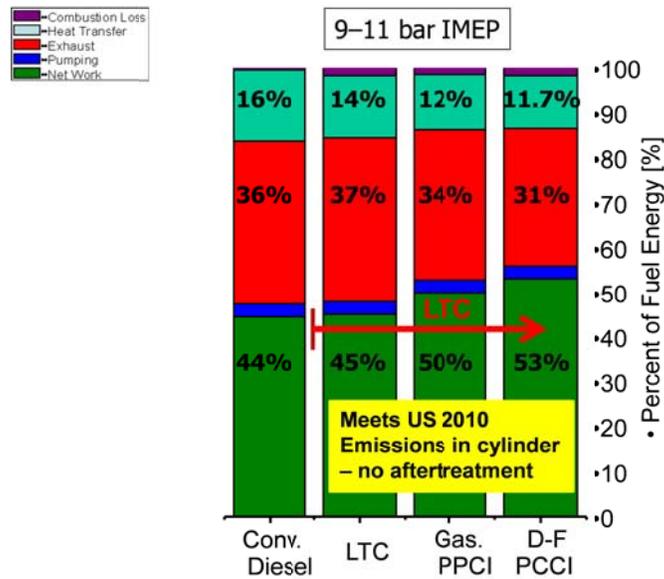


Figure 5, Comparison of measured thermal efficiencies at 9 bar IMEP obtained on ERC Caterpillar SCOTE engine for conventional diesel, low temperature, gasoline partially premixed and diesel/gasoline dual fuel combustion. (Adapted from [10])

Figure 5 shows a First Law energy balance for a heavy duty single cylinder engine operating at moderate load using conventional diesel combustion and different approaches of “flameless” combustion. All of the stack plots to the right of the conventional diesel energy partitioning are what I am referring to as low temperature combustion. In the Figure, the LTC column just to the right of the conventional diesel is “flameless” combustion with diesel fuel. Gas PPCI is “flameless” combustion using gasoline compression ignition with varying degrees of premix, which is controlled by

multiple injections of fuel during the compression stroke. And, D-F PCCI is “flameless” combustion with a premixed gasoline base charge followed by one or more smaller injections of diesel fuel during the compression stroke. All of the cases labeled LTC with the red arrow, have engine out emissions that are below 2010 standards.

Further study of Figure 5 shows the trade-off between the different energy partitioning that result from the reduction of combustion temperatures achieved through Low Temperature Combustion. As the combustion process is moved into LTC regimes, the work out of the cylinder increases with an attendant decrease in the heat transfer and energy thrown away in the exhaust. The upper most energy partition, combustion loss, represents incomplete combustion and not irreversibilities of combustion. In a First Law presentation like this irreversibilities are not discernible. The reason for the shifts in the energy partitioning yielding more work out is what was explained in the beginning of this paper.

The reason for the differences in work output for the different LTC combustion modes is related to the fuels. The column in the Figure labeled LTC uses diesel fuel. To introduce the fuel, get it to vaporize and mix to an appropriate level of homogeneity such that the auto-ignition process proceeds to ignition at an appropriate time requires very different intake conditions and fueling strategies than to accomplish that same sequence of processes for the different fuels – gasoline and gasoline/diesel. The sequence of processes that need to be accomplished is the same for each of the three generic LTC combustion modes shown in the Figure, however, depending on the fuel’s auto-ignition characteristics and its physical properties the methods employed to achieve these processes were different.

Brief Overview of LTC Activities

Herein lays the challenge with low temperature combustion. The in-cylinder conditions, (temperature, pressure and oxygen concentration), the compression process itself, and the manner in which the fuel is introduced into the cylinder will be intimately tied to the auto-ignition characteristics of the fuel. And, what is done to manipulate these parameters is done significantly before the point in the cycle at which auto-ignition is desired. To be successful one has to actively manipulate and intervene in the auto-ignition reactions of the fuel air mixture. Significant progress has been and continues to be made in besting these challenges.

LTC combustion processes are being actively studied and developed throughout the world. Research at Toyota [11, 12, 13, and 14] has explored pre-mixed diesel combustion modes. Nissan Diesel uses LTC as part of the operating map for engines that are currently in the market. Nissan refers to the combustion as Modulated Kinetics, or MK, combustion [15]. In MK combustion the swirl level in the cylinder is increased, the EGR level is raised and the high pressure injection is significantly retarded. The combination of the low oxygen concentration from the high EGR, the increased mixing from the high swirl and the retarded injection results is a somewhat homogeneous charge that auto-ignites with volumetric energy release. Nissan uses MK combustion for NOx

and particulate control. The retarded injection timing necessary to achieve MK combustion results in a detriment in fuel consumption, but it is not as bad as one might guess because the energy release rate of the MK combustion is more rapid than typical mixing controlled conventional diesel combustion.

Toyota's UNIBUS (uniform bulk combustion system) [14] uses early injection with low temperatures and high EGR to extend the ignition delay sufficiently to achieve the requisite mixing for LTC. However the low temperatures and high EGR negatively affects combustion stability.

Kalghatgi et al. [16, 17] found using gasoline that the high resistance to auto-ignition of lower CN fuels allows more mixing time prior to combustion, thus lowering NO_x and PM emissions. They also demonstrated that start-of-combustion timing could be controlled with suitably timed dual injections, and that the apparent heat release rate could be lower than diesel Homogeneous/Premixed Charge Compression Ignition (HCCI/PCCI) at similar loads. The use of timed multiple injections for combustion phasing controlled was also proposed by Marriott and Reitz [18].

Hanson et al. [19] demonstrated the feasibility of using gasoline in heavy-duty compression ignition engines with optimal single injections and moderate EGR levels. Their results showed that 2010 emissions levels could be met in-cylinder, while maintaining low fuel specific fuel consumption, reasonable pressure rise rates, and existing engine and fuel injection hardware. The simultaneous reduction of PM and NO_x obtained with partially premixed combustion (PPC), along with the ability for combustion control is very desirable because it allows low emissions within a larger operating range than with traditional pre-mixed combustion regimes, while also increasing the engine efficiency.

Experiments performed by Bessonette et al. [20] with a variety of fuels suggested that the best fuel for HCCI operation may have auto-ignition qualities between that of diesel and gasoline. Using a compression ratio of 12:1 and a fuel with a derived cetane number of ~27 (i.e., a gasoline boiling range fuel with an octane number of 80.7), they were able to extend the HCCI operating range to 16 bar BMEP – a 60% increase in the maximum achievable load compared to operation using traditional diesel fuel. Furthermore, their results showed that low load operation (below 2 bar BMEP) required a derived cetane number of ~45 (i.e., traditional diesel fuel).

In addition to the challenge of developing a robust control strategy for LTC, on which impressive progress is being made, achieving high load is a major issue. This challenge is fundamental. The goal of LTC is to achieve volumetric energy release via auto-ignition. This is the same as knocking combustion. To moderate the rates of pressure rise the air fuel mixture in the cylinder is diluted. To reach high load more fuel must be introduced into the cylinder, which constrains the extent to which dilution can be used to moderate the rate of pressure rise. Typically as LTC is pushed towards higher load excessive rates of pressure rise become the limiting metric, and the operational window for LTC becomes very narrow.

The work of Dec et al., summarized in Figure 6, shows the typical profile of the narrowing of the operating range as load is increased. The data shown in the figure give the temperature range for gasoline homogeneous charge compression ignition, LTC, as the load is increased - shown as the fuel/air equivalence ratio. At each load the LTC regime is bounded on a low temperature side by unstable combustion, and is bounded on a high temperature side by excessive rates of pressure rise, the ringing limit. As the load is increased the operating temperature window becomes narrower, until there is a load at which acceptable LTC cannot be obtained.

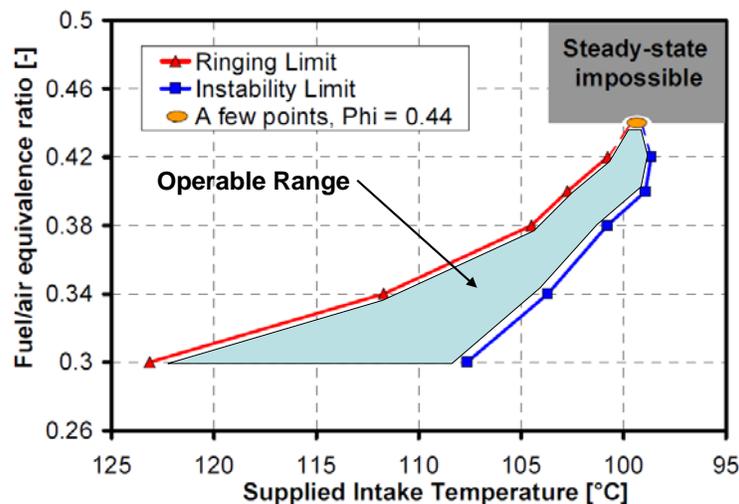


Figure 6, As combustion phasing sensitivity to inlet temperature increases at higher load, Dec et al. hypothesize that steady state operation is impossible at the high load limit due to a convergence of excessive ringing and instability limits [21]

The same research group at Sandia [22] demonstrated that the upper load limit in a medium duty diesel engine could be increased from 11 bar IMEP for homogeneous charge to 13 bar IMEP when using controlled fuel stratification.

Several of the references cited above in the general description of LTC, [10, 16, 17, 18, and 19] were also addressing the issue of raising the load limit of LTC by controlling the relative reactivity of the air fuel mixture in the cylinder through the use of two fuels. The activities are extensive. The work of Ra et al. [23] has shown through an experimental program, that was guided by detailed CFD, that a load of 17 bar IMEP could be achieved in a single cylinder engine matching the geometry and hardware of a 4 cylinder, 1.9 L light duty diesel engine. At this operating condition the fuel consumption and emissions were low: $isfc = 173 \text{ g/kW-h}$, $NO_x = 0.15 \text{ g/kg-f}$, and $PM = 0.1 \text{ g/kg-f}$. This was accomplished with triple injection of a single fuel, an 87 ON gasoline.

The above is only a superficial coverage of the vast work taking place worldwide addressing the issues of LTC control and expanding its operating range. Many laboratories that are doing excellent work are not mentioned in the above overview. For

example Lund University has extensive activity in this area and has contributed significantly to the technical communities understanding of LTC. Reference 24 is but one of many contributions to the literature in which they are exploring optimal fuel characteristics and methods of expanding the operating regime. To all the researchers/colleagues who I slighted by not referencing their work, I apologize; omission of recognition was driven by space limitation and not lack of importance.

Gas Exchange and Engine System Control for LTC

The above overview of results shows that the in-cylinder conditions can be sufficiently controlled to achieve LTC over a reasonable portion of the engine's load and speed map. In fact the engine manufacturers participating in the DOE Super Truck Program have integrating LTC processes into their proposed engine maps as an important component of meeting the efficiency and emissions goals of the program.

However it is also clear that controlling the temperature, pressure, oxygen concentration, in-cylinder fluid mechanics, and fuel introduction processes is critical. This puts more demands on the gas exchange and control system of the engine. Because of the complex chemistry of auto-ignition and its subtle variations with fuel types, it seems that active in-cylinder combustion sensing will probably be required for successful integration of LTC into the operational map of the engine in a vehicle. For gas exchange; boosting systems, heat exchange processes, and EGR system performance will be critical. And finally, exhaust gas aftertreatment systems will probably still be needed and they will need to operate at lower exhaust temperatures. This is a thermodynamic principle. As the engines get more efficient the exhaust temperature will be reduced.

Summary

The above article has argued that there is fundamental thermodynamic underpinning for the case that Low Temperature Combustion can lead to improved efficiency from internal combustion engines. Unfortunately when we use combustion to release the chemical energy in the fuel as part of the process of producing work we must accept that approximately 20 percent of the fuel's availability will be destroyed. We are fortunate in that even though the availability destruction during combustion increases with lower combustion temperatures, within the range of temperatures experienced in engines the increase in availability destruction with Low Temperature Combustion is small relative to that caused by typical flame propagation. The thermodynamic benefits of the low in-cylinder temperature offset this detriment of increased availability destruction.

If in-cylinder combustion temperatures can be kept low, the ratio of specific heats does not decrease as much as it does for more typical combustion processes involving flame propagation. The relatively larger ratio of specific heats gives the benefit of more work extraction during the expansion process, which in turn reduces the available energy at exhaust valve opening. In addition the lower in-cylinder temperatures reduce heat transfer from the cylinder which has a double benefit. Not only is less energy lost via heat transfer, but the availability per unit of energy lost is lower as well.

Thus Low Temperature Combustion maximizes the work gained from the expansion process which is highly desirable because the compression and expansion processes in the engine are highly efficient.

LTC is in essence controlled knock, and relies on the auto-ignition chemistry of the fuel. Regardless of the fuel, the underlying approach to achieving acceptable LTC is the same. One wants to get the fuel vaporized and partially premixed such that when the auto-ignition chemistry reaches the point of ignition the energy release is volumetric. There needs to be sufficient inhomogeneity of the mixture within the combustion chamber that the entire mixture does not auto-ignite all at once. This inhomogeneity can be in temperature, air fuel ratio, or degree to which the local mixtures have kinetically traversed their auto-ignition pathway. Depending on the volatility and ignition characteristics of the fuel, the pathway to achieving this fuel-air distribution can be very different.

LTC leverages the advantages of classic diesel combustion, however integrating it into an engine system brings new challenges. Because we wish to establish a somewhat uniform fuel air mixture which undergoes sequential auto-ignition, our last control input often occurs significantly in advance of the ignition time for optimal combustion phasing. This makes combustion control over a range of speeds and loads a challenge. Very light load is a challenge because it requires the auto-ignition of a very dilute mixture of fuel and air. Conversely, achieving heavy load without excessive rates of pressure rise is a challenge because now you need to auto-ignite a fuel air mixture with the maximum amount of fuel in the cylinder.

Tremendous progress has been made in controlling LTC auto-ignition processes within the cylinder, and it has become common for developers to establish an acronym which describes the method being used to establish and control the LTC. Expanding these accomplishments to incorporate LTC into the powertrain of a vehicle will require integrating an understanding of the fundamental processes of the fuels' auto-ignition characteristics and how these couple with the in-cylinder thermodynamic conditions into the engine controls system. This probably necessitate some sort of in-cylinder sensing for dynamic control; and the gas exchange systems of the powertrain – the boosting, EGR, heat exchange, and charge motion control subsystems, will play a critical role as well.

References:

1. *Real Prospects for Energy Efficiency in the United States*, report by the National Academy of Sciences, Washington, D.C., 2009.
2. Heywood, J.B., *Internal Combustion Engine Fundamentals*, McGraw Hill, Inc., 1988, ISBN 0-07-028637-X
3. O'Hayre, R.P, Cha, S-W, Colella, W.G, Prinz, F.B., *Fuel Cell Fundamentals*, John Wiley and Sons, Inc. 2009, ISBN978-0-470-25843-9
4. Edo, T., and Foster, D.E., *VI International Symposium on Alcohol Fuels Technology*, Ottawa Canada, 1984

5. C. D. Rakopoulos and E. G. Giakoumis, "Second-law analysis applied to internal combustion engine operation," *Progress in Energy and Combustion Science*, 32, 2–47 (2006).
6. N. Lior and G. J. Rudy, "Second-Law Analysis of an Ideal Otto Cycle," *Energy Conversion and Management*, 28(4), 327–334 (1988).
7. R. J. Primus, K. L. Hoag, P. F. Flynn, and M. C. Brands, Appraisal of Advanced Engine Concepts Using Second Law Analysis Techniques, SAE Technical Paper 840032
8. C. S. Daw, R. L. Graves, R. M. Wagner, and J. A. Caton, *Report on the Transportation Combustion Engine Efficiency Colloquium Held at USCAR*, March 3–4, 2010, ORNL/TM-2010/265
9. Druecke, B.C., Foster, D.E., Klein S.A., Daw, C.S., Chakravarthy, V.K., and Graves, Second Law Analysis of Constant Temperature Combustion", Central States Section Combustion Institute, Chicago, IL, March 2006 , also MSME University of Wisconsin – Madison 2006
10. Kokjohn, S., Hanson, R., Splitter, D, and Reitz, R.D., "Experiments and Modeling of Dual Fuel HCCI and PCCI Combustion Using In-Cylinder Fuel Blending," Powertrains Fuels and Lubricants Meeting, SAE Technical Paper 2009-01-2647
11. Akihama, K., Takatori, Y., Inagaki, K., Sasaki, S., Dean, A., 2001, "Mechanism of the Smokeless Rich Diesel Combustion by Reducing Temperature," SAE Technical Paper 2001-01-0655
12. Shimazaki, N., Tsurushima, T., Nishimura, T., 2003, "Dual Mode Combustion Concept with Premixed Diesel Combustion by Direct Injection near Top Dead Center," SAE Technical Paper 2003-01-0742
13. Minato, A., Tanaka, T., Nishimura, T., 2005, "Investigation of Premixed Lean Diesel Combustion with Ultra High Pressure Injection," SAE Technical Paper 2005-01-0914
14. Okude, K., Mori, K., Shiino, S., Moriya, T., 2004, "Premixed Compression Ignition (PCI) Combustion for Simultaneous Reduction of NO_x and Soot in Diesel Engine," SAE Technical Paper 2004-01-1907
15. Kimura, S., Osama, A., Ogama, H., Muranaka, S., 1999, "New Combustion Concept for Ultra Clean and High-Efficiency Small DI Diesel Engines," SAE Technical Paper 1999-01-3681
16. Kalghatgi, G. T. and Risberg, P. and Ångström, H.-E., "Partially Pre-Mixed Auto Ignition of Gasoline to Attain Low Smoke and Low NO_x at High Load in a Compression Ignition Engine and Comparison with a Diesel Fuel", SAE Technical Paper 2007-01-0006.
17. Kalghatgi, G. T. and Risberg, P. and Ångström, H.-E., "Advantages of fuels with high resistance to auto-ignition in late-injection, low-temperature, compression ignition combustion", SAE Technical Paper 2006-01-3385.
18. Marriott, C.D., and Reitz, R.D., "Internal Combustion Engine Using Premixing with Combustion of Stratified Charges," US Patent 6668789, 12/30/2003.
19. Hanson, R., Splitter, D., and Reitz, R.D., "Operating a Heavy Duty DIC_I Engine

- with Gasoline for Low Emissions," SAE Technical Paper 2009-01-1442, 2009.
20. Bessonette, P. W., Schleyer, C. H., Duffy, K. P., Hardy, W. L. and Liechty, M. P., "Effects of Fuel Property Changes on Heavy-Duty HCCI Combustion", SAE Technical Paper 2007-01-0191, 2007.
 21. Sjoberg, M., Dec, J., Babajimopoulos, A., Assanis, D., 2004, "Comparing Enhanced Natural Thermal Stratification Against Retarded Combustion Phasing for Smoothing of HCCI Heat-Release Rates," SAE Technical Paper 2004-01-2994
 22. Dec, J., Yang, Y., Dronniou, N., 2011, "Boosted HCCI – Controlling Pressure-Rise Rates for Performance Improvements using Partial Fuel Stratification with Conventional Gasoline," SAE Technical Paper 2011-01-0897
 23. Youngchul Ra, Paul Loeper, Michael Andrie, Roger Krieger, David Foster, Rolf Reitz, and Russ Durrett, "Gasoline DICI Engine Operation in the LTC Regime Using Triple- Pulse Injection", SAE Technical Paper 2012-01-1131
 24. Lewander, M., Johansson, B., and Tunestål, P., "Investigation and Comparison of Multi Cylinder Partially Premixed Combustion Characteristics for Diesel and Gasoline Fuels," SAE Technical Paper 2011-01-1811